

## Rapid Evaluation of Research Proposals Using Aspen Plus

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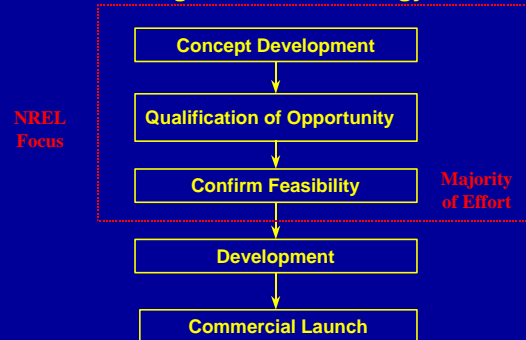
## NREL

- National Renewable Energy Laboratory
- Operated under the Direction of the US Department of Energy
- Multiple Programs in Renewable Energy Area
- Specific Area of Interest, Biofuels
  - Production of Fuels from Lignocellulosic Biomass
  - Specifically using Biological Processes

## Our Business

- Develop Technology to Enable the Competitive Production of Ethanol from Lignocellulosic Biomass
- How do we do that?
  - Sponsor Research on the Most Promising new Technologies
    - Both at NREL and at Universities and Industries
- Which Projects should be Funded?
  - Use a modified “Stage-Gate” Methodology to Select

## Stage Gate Methodology



## How Do You Determine What Research Projects to Fund?

- Stage 2 is a Preliminary Investigation (1 man-month max)
- Stage 3 Is Where NREL Funds Research
- To Pass Gate 2 The Project Must Meet:
  - Subjective Information
    - Fit in the Strategy of the Base Process
    - Be Feasible
    - Reasonable Goals and Show-Stoppers
    - Reasonable Time Frame and Resource Requirements
  - Objective Information
    - Be Economically Attractive as Compared to the Base-Case

## Rapid Economic Evaluation Allows Management to:

- Have Some Objective Information to Make Go/No Go Decisions
- Prioritize Seemingly Go Projects Based on Economic Impact

## Types of Process Economics Performed for NREL Biofuels

- **Absolute Cost of Biomass to Ethanol Conversion**
  - Useful for Market Penetration Studies
  - Required for Site Specific Project Feasibility Studies
- **Incremental Cost Improvements of Research Proposals**
  - Use as Objective Information in Stage Gate Screening
  - More Accurate than Absolute Costs

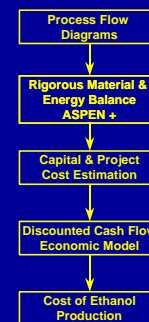
## Rigorously Develop a Base-Case

- **Feed - Woodchips or Agricultural Waste**
  - 2000 dry Tons/day
- **Production - Fuel Grade Ethanol**
  - 70MM+ gallons / year
- **9 Process Areas**
  - 23 PFD
  - 181 Costed Unit Operations
- **Research Ideas Modeled as Process Alternatives**

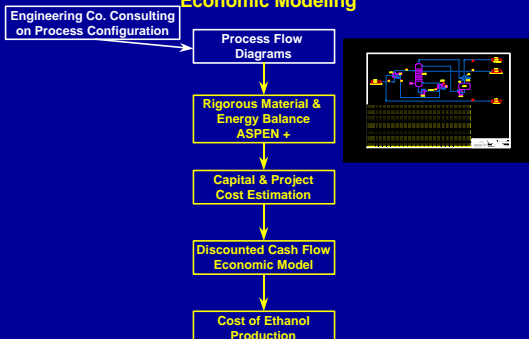
## Base ASPEN Plus Model

- 147 Unit Operations
- 59 Components
- 217 Material Streams
- 211 Heat and Work Streams
- 60 Control Blocks (Design-Spec & Fortran)

## NREL's Approach to Process Design and Economic Modeling

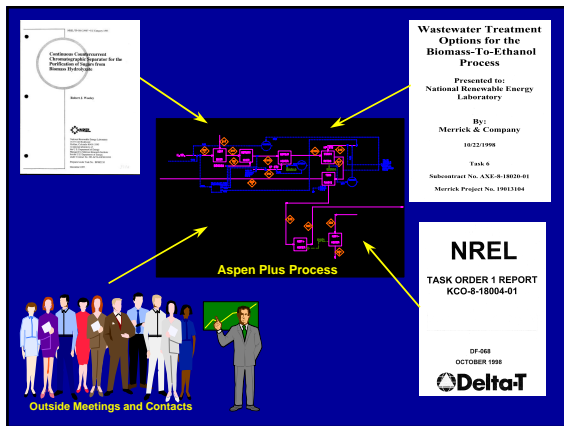


## NREL's Approach to Process Design and Economic Modeling



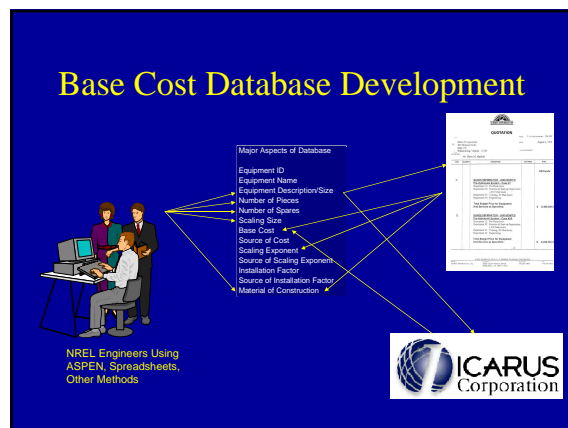
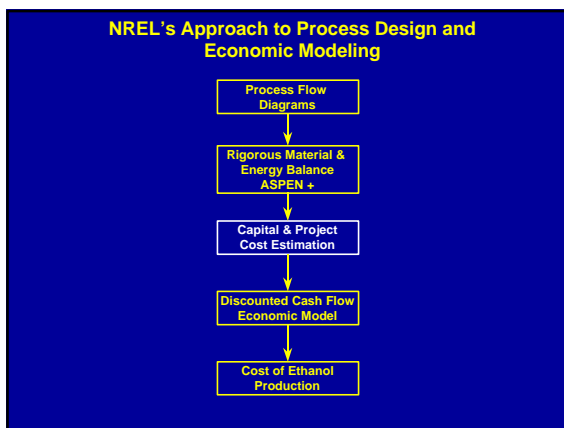
## Why Use a Process Simulator? (ASPEN Plus)

- Rigorous Thermodynamic Models Built In
- Rigorous Unit Operation and Recycle Convergence Built-In
- Easy Translation of Complex Processes with Solids into Included Unit Operation Blocks
- Easily Customizable when Necessary
- Self Documenting
- Easily Understandable, Widely Used in the Industry
- Commercially Supported



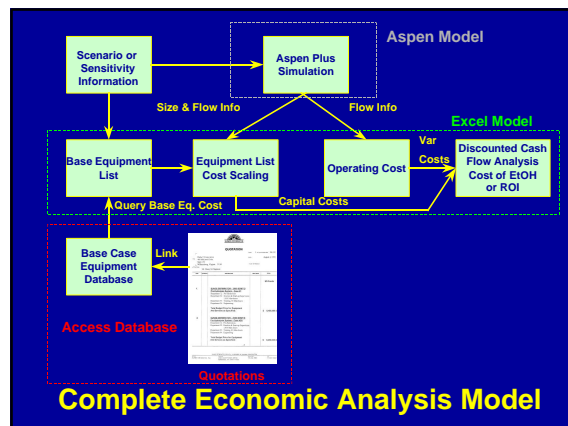
## Approach to Detailed Process Modeling

- Use Detailed Modeling to Support and Interpret Experimental Work
  - Fortran, MatLab, Aspen/Plus, Aspen/SP, Scientist, Excel, Others
- Translate Experimental Work and Detailed Modeling into “Simpler” Forms
- Use a Less Detailed ASPEN Model to Describe the Entire Integrated Process



### Important Ancillary Information in Cost Database

- Scaling Exponent
- Scaling Item from Aspen
  - Identification of Item
    - Flow
    - Size
  - Base Value
  - Units



## Do Not Redesign and Cost Each Alternative

- Scaling of Aspen Information in to Costs
  - Base Information from Access Database
    - Base Cost
    - Base Variable
    - Base "Size"
  - Use Excel Spreadsheet to Scale Costs
  - Use Information from Aspen on New "Size"
    - Flow
    - Calculated Size, e.g., Column Diameter
    - Heat Duty, e.g, No  $\Delta T$  Changes
    - Calculated Area, e.g., HX from Fortran

## Extract Information from ASPEN Plus

- Consolidate in Sensitivity Block
- Extract to Excel Look-up Table
  - From GUI Use Paste-Link
  - From Input File Mode Use VB-Summary File Tool Kit

## Extract Information from MS Access Database Where PFD Like 'PFD-P100\*'

ASSOCIATED PFD	EQUIP NUM	NUM REQ.	NUM SPARE	NUM REQUIRED VAR	PROCESS ITEM FOR SCALING	BASE FOR SCALING	BASE COST	SCALE EXP
PFD-P100-A302	A-300		0	INUMSSFA			19676	
PFD-P100-A302	A-301	1	0		STRM0304	41777	12551	0.51
PFD-P100-A302	A-304	2	0		STRM0304	41777	11700	0.51
PFD-P100-A302	A-305	2	0		STRM0304	41777	10340	0.51
PFD-P100-A302	A-306	1	0		STRM0502	381700	10100	0.51
PFD-P100-A302	H-302	3	0		AREA0302	3765	25409	0.78
PFD-P100-A302	H-304	1	0		QSDFO301	38339	3300	0.83

## ASPEN Plus Simulation Information Transferred to Excel

Variable Name	Value	Units
AREA0302	3,700	
DIAMD501	3.89	METER
INUMSSFA	34	
NUMRCENT	3	
QRFD0502	986,470	CAL/SEC
QSDFO301	35,069	CAL/SEC
STRM0303	35,086	KG/HR
STRM0304	37,997	KG/HR
STRM0502	380,206	KG/HR
WRKWOTOL	-41,651	KW
Total Number of Items Retrieved: 154		

Variable Names are in Alphabetical Order for Excel "Look-up" Table

Calculated in FORTRAN in ASPEN

Unit Operation Variable

Heat Stream Duty

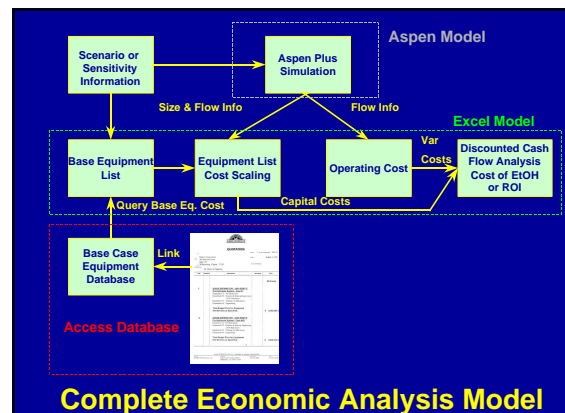
Material Stream Flow

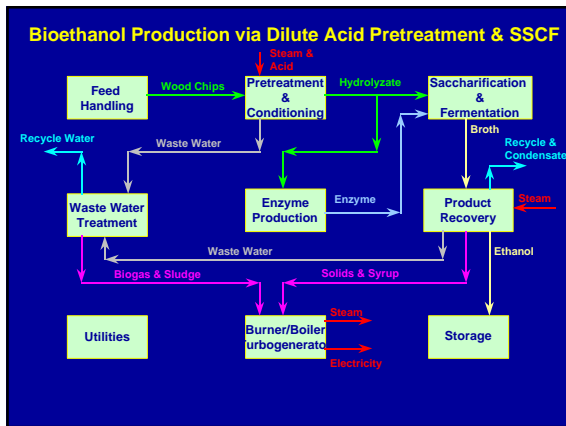
Work Stream Power

## Equipment Cost Scaling in Excel

Equip No.	No. Req'd	No. Spare	No. Req. Variable	Scaling Item	Scaling Item Value	New Item Value	Original Equip Cost (per unit)	Total Equip Cost	Scaling Exp.	Scaled Cost
A-300	34			INUMSSFA			\$ 19,676	\$ 668,984		\$ 668,984
A-301	1			STRM0304	41,777	37,997	\$ 12,551	\$ 12,551	0.51	\$ 11,968
A-304	2			STRM0304	41,777	37,997	\$ 11,700	\$ 23,400	0.51	\$ 22,295
A-306	1			STRM0502	381,700	380,206	\$ 10,100	\$ 10,100	0.51	\$ 10,080
H-302	2	1		AREA0302	3,765	3,700	\$ 25,409	\$ 76,227	0.78	\$ 75,202
H-304	1			QSDFO301	38,339	35,069	\$ 3,300	\$ 3,300	0.83	\$ 3,065

ASPEN PLUS Value - Look-up From ASPEN Plus Link  
 MS Access Database Value - Look-up from MS Access Link  
 Calculated Value  
 User Entered Specification





## Evaluation of Research Ideas

- Understand Research Idea
  - Scientist Explains Idea to Engineer
- Anticipate Expected Range of Research Results
- Transform Idea and Expected Results into Modifications to Process Model
- Add New Equipment Estimates
- Determine Cost Differential due to Modification

## Total Numbers of Sensitivities For 1 Base Process

Pretreatment	9
Detoxification	14
Fermentation	30
Enzyme Production	14
Waste Treatment	4
Utilities	2
Economics	2
Total	74

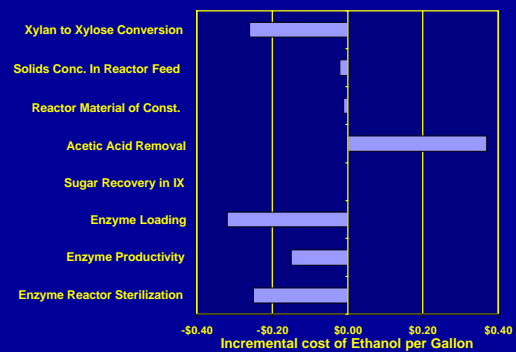
## Example Process Alternatives

Process Area	Process Parameter
Pretreatment	Xylan to Xylose Conversion
Pretreatment	Solids Concentration in Feed
Pretreatment	Reactor Material of Construction
Pretreatment	Acetic Acid Removal
Pretreatment	Sugar Recovery in IX
Enzyme Production	Enzyme Loading
Enzyme Production	Enzyme Productivity
Enzyme Production	Sterilization

## Total Number of Assessments

- 3 base Processes
- High and Low for Each Sensitivity
- Over 400 Sensitivities

## Incremental Economic Impact of Research Alternatives



## Result

- Develop Base-case in Detail
  - Documents Sensitivities, Eliminates Repeated Work
- Scale Process Options off Base-case Detailed Economics
- Parameter and Configuration Changes to Aspen
- Minor Equipment Cost Modifications for Individual Alternatives
  - Only if new process is significantly different than Base
- Cost Impact of Each Alternative